



CO₂ capture. Two new structures in the 2-amino-2-methyl-1-propanol (AMP) – water – CO₂ system

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basis for studying more transition metal combinations. Future plans also entail *in operando* studies of structural changes during battery charge and discharge.

[1] M.H. Han, E. Gonzalo, G. Singh and T. Rojo *Energy Environ. Sci.*, 2015, 8, 81. [2] C. Delmas, C. Fouassier and P. Hagemuller *Physica B+C*, 1980, 99, 81.

Keywords: Batteries, Na_xMO_2 , Layered structures

MS05-P04 Study and Characterization of a Polypropylene and Tire Powder Composite for Use in the Automotive Industry

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The development of the automotive industry in the twentieth century has increased the production of motor vehicles, generating an increase of the national fleet, and the consumption of tires reached staggering numbers. By this reason, the amount of solid wastes generated and deposited in the environment has grown considerably. In order to minimize the impacts arising from this deposition, some environmental agencies have created resolutions to ensure proper disposal of scrap materials. [1]. At the end of its service life, the wasted tires, without shooting conditions or reforms, are difficult to recycle because the vulcanization process makes the material infusible and of difficult processability. When discarded in inappropriate locations, tires may serve as a medium for the development of disease vectors besides representing risk of fire, polluting the air with toxic fumes – containing pollutants such as carbon and sulfur – as well as releasing oil, which can contaminate the water table [2]. In order to reduce the amount sent to the environment and to generate an appropriate production cycle, the wasted tire was used as reinforcement in a polymeric matrix to be applied to the engine encapsulation of commercial vehicles. It is intended to provide a reduction of the piece weight and thus the vehicle, optimizing fuel consumption and reducing the emission of pollutants; additionally, it ensures the minimization of noise pollution through the noise attenuation by the composite. Acoustic analysis of transmission loss and external noise were performed to verify whether the material complies with the limits specified by the resolutions. The X-ray powder diffraction analysis was fulfilled to identify and quantify the different phases that composing the material.

[1] Associação Nacional das Indústrias de Pneumáticos - ANIP. – “Produção na Indústria Brasileira e Reciclagem de Pneus”, ANIP, São Paulo, 2010. Disponível em: <<http://www.anip.com.br>>. Acesso em: 10 de julho de 2015. [2] Laganinhos C. A., Tenório J. A. S. *Polímeros: Ciência e Tecnologia*, 2008, 18, 106.

Keywords: tire powder, X-ray diffraction, engine encapsulation

MS05-P05 CO₂ capture. Two new structures in the 2-amino-2-methyl-1-propanol (AMP) – water – CO₂ system

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Energy production and transportation is responsible for more than 60 % of our CO₂ emission. In particular coal-fired power plants are big contributors. However, these large scale facilities offer the possibility to effective CO₂ capture through post-combustion processes. There are several options for such CO₂ capture. The problem is to make the absorption/desorption processes energetically and thereby economically viable. One process under investigation involves alkanoamines as absorbents in aqueous solutions. In these systems CO₂ is captured either by carbonate and/or carbamate formation. We have studied the 2-amino-2-methyl-1-propanol (AMP) and the AMP-water phase diagram and its ability for CO₂ capture. The first crystal structure in the AMP – water system has been solved from powder diffraction data: AMP trihydrate (triclinic, P-1, a = 6.5897(3), b = 6.3997(2), c = 6.3399(2) Å and α = 92.407(3), β = 113.345(3) and γ = 94.706(2) °). In the AMP – water CO₂ system two structures, a carbamate, AMPH-AMPCO₂ and a carbonate, (AMPH)₂-CO₃ are known [1]. In this work we solved a new structure from powder diffraction data, AMPH-

HCO₃ hydrate (monoclinic, I2/a, a = 21.8522(7), b = 6.2149(15), c = 12.1300(3) Å, β = 104.036(16) °) readily formed when using <40 at% AMP in water.

[1] Barzagli F., DiVaira M., Mani F. and Peruzzini M. *ChemSusChem*, 2012, 5, 1724.

Keywords: carbon capture, 2-amino-2-methyl-1-propanol

MS05-P06 Metal Halide Hybrid Materials Topology & Photonics

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Actually, Metal Organic Frameworks (MOFs) are dethroning zeolites in hydrogen storage, greenhouse gas capture, drugs field, catalysis, energy storage, etc... In particular, in the photonics field, self-organized lead halide organic-inorganic hybrids exhibit confined excitons in one- two- or three- dimensional secondary building unit (SBU) network with corner, edge, face or mixed mode sharing topology.

Generally, the HOMO-LUMO energy gaps of the organic part are higher than that of the inorganic moiety. Therefore, the electronic structures of these compounds can be regarded as a self organized multiple quantum-dot -well or bulk structures. The high contrast in dielectric constants between the organic and inorganic parts strengthens the interaction between an electron and a hole in a stable exciton with a strong binding energy that can be set free as photoluminescence emission at room temperature.

Several kinds of parameters rule the photonic properties of the lead halide hybrids. On the one hand, in the inorganic part: the Bohr radius of the exciton, the exciton band gap, the anionic secondary building unit dimensionality, the octahedral connection topology... etc, and the length of the alkyl chain, the steric encumbrance, the structural flexibility on the other hand in the organic moiety. The long-term stability under illumination, the temperature and some other factors can be decisive on the stability and the optical behaviours of these MOFs.

Keywords: halides, topology, crystal structure, luminescence, exciton

MS05-P07 Determination of amphibole asbestos fibres by powder X-ray diffraction and comparison with other used methods (IR, optical microscopy, electron microscopy)

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Our previous work dealt with actinolite occurrence in solid fraction of ambient aerosol in Pilsen basin (Western Bohemia) and its source apportionment. Our technology consisted of collection dust particles on glass fibre (non-diffracting) filters. The filters were worked up directly by X-ray powder diffraction using parallel-beam geometry (like thin layer). Semiquantitative analysis were done by „Reference Intensity Ratio“ (RIR) method [1] used previously i.e. for XRD analysis of atmospheric dust in several other places [2], [3]. The aim of this work is to compare diffraction methods with other methods, widely used for asbestos fibers detection and determination. For this purpose we have used artificially prepared samples with defined actinolite content. The samples were transformed into aerosol using tubular aerosol suspension chamber according Davis [1] and collected on filters. The filters were then analysed by XRD using parallel beam geometry, IR spectroscopy and electron microscopy. Additionally, a few naturally obtained samples were studied too. As a conclusion, the results from different methods were compared and suitability of diffraction method was discussed.

[1] B.L. Davis, Reference Intensity Method of Quantitative X-Ray Diffraction Analysis (Davis Consulting, Rapid City, 1988). [2] B.L. Davis *Atmospheric Environment*, 1984, 18, 2197. [3] B.L. Davis and J. Guo *Atmospheric Environment*, 2000, 34, 2703.

Keywords: asbestos, XRD quantitative analysis, IR spectroscopy and microscopy